Dislocation nucleation in nanoporous single-crystal nickel: molecular dynamics simulations and analytical modelling

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Nanovoids are commonly observed in metals under extreme environmental conditions, resulting from vacancy condensation. This is the case, for example, with nickel-based alloys used in nuclear applications, where nanovoids are common radiation-induced defects ranging in size from a few nanometres to several tens of nanometres, well below the grain size. The mechanical behaviour of nanoporous single crystals has been extensively studied in the literature. Most studies have focused on uniaxial loading conditions using molecular dynamics (MD) simulations. Fewer studies have assessed the effect of triaxial loading conditions, which are more relevant for applications, or proposed analytical criteria to recover numerical results. In this study, MD simulations were performed to investigate the mechanical behaviour of a perfect single-crystal of nickel containing pre-existing nanovoids. The focus was on the onset of plasticity, which is defined by the nucleation of the first dislocation. The effects of mechanical loading paths, crystallographic orientations, void sizes and shapes were systematically investigated, leading to macroscopic yield surfaces. The results reveal a significant effect of crystal orientation on the material's yield surface, indicating a strong anisotropic mechanical response, as well as an effect of void shape. A detailed analysis of dislocation nucleation events also revealed that the maximum resolved shear stress remained relatively constant across all cases. Based on Eshelby theory and the existence of a critical resolved shear stress, a semi-analytical model is thus proposed to describe dislocation nucleation in nanoporous single crystals. Good agreement was observed between the MD results and the proposed model.